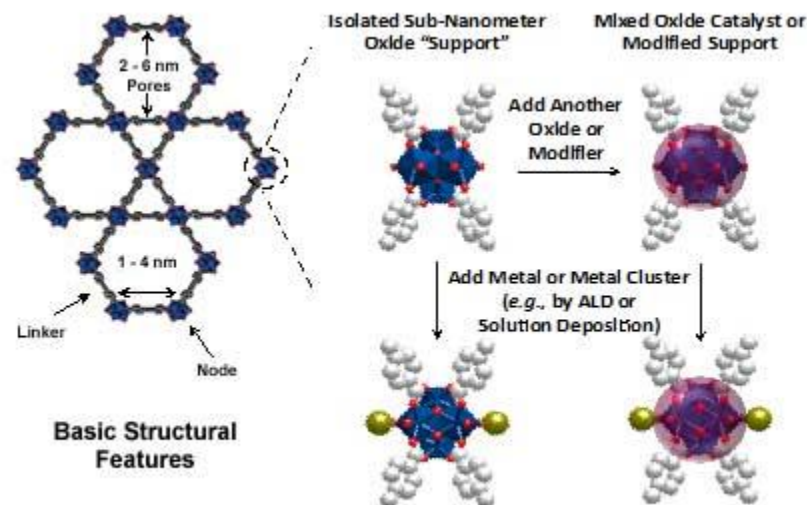


Inorganometallic Catalyst Design Center (ICDC)

Laura Gagliardi (University of Minnesota)

ICDC is devoted to guiding the discovery of superior catalysts by integrating computational modeling with experiments in well-defined systems that are amenable to high-throughput search and discovery methods.

<http://www.chem.umn.edu/icdc/>



RESEARCH PLAN

ICDC designs a new class of catalysts consisting of inorganometallic clusters supported by metal-organic frameworks. ICDC computationally predicts such cluster catalysts for conversions of natural gas into methanol and oligomers, with new quantum and classical simulation techniques. The coupling between the experimental and the theoretical efforts ensures that the discovery of these novel materials and the understanding of their properties occurs through a truly iterative theoretical/experimental loop.



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